

## 1-Benzoyl-3-(naphthalen-1-yl)thiourea

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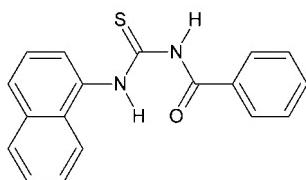
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Key indicators: single-crystal X-ray study;  $T = 173\text{ K}$ ; mean  $\sigma(\text{C}-\text{C}) = 0.004\text{ \AA}$ ;  $R$  factor = 0.062;  $wR$  factor = 0.135; data-to-parameter ratio = 16.9.

In the title compound,  $\text{C}_{18}\text{H}_{14}\text{N}_2\text{OS}$ , the dihedral angle between the mean planes of the 3-naphthyl and 1-benzoyl rings is  $20.7(1)^\circ$ . The crystal packing is stabilized by weak  $\text{N}-\text{H}\cdots\text{S}$  interactions. Intramolecular  $\text{N}-\text{H}\cdots\text{O}$  and  $\text{C}-\text{H}\cdots\text{O}$  hydrogen bonding is also observed.

### Related literature

For the biological activity of thiourea in medicinal chemistry, see: Saeed *et al.* (2009, 2010a,b); Maddani & Prabhu (2010). For the use of thiourea derivatives in organocatalysis, see: Jung & Kim (2008) and for their use as curing agents for epoxy resins, see: Saeed *et al.* (2011). For the use of thioureas as ligands in coordination chemistry, see: Burrows *et al.* (1999); Henderson *et al.* (2002); Schuster *et al.* (1990). For the pesticidal activity of acyl thioureas, see: Che *et al.* (1999). For standard bond lengths, see Allen *et al.* (1987).



### Experimental

#### Crystal data

$\text{C}_{18}\text{H}_{14}\text{N}_2\text{OS}$	$V = 1455.2(4)\text{ \AA}^3$
$M_r = 306.37$	$Z = 4$
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation
$a = 9.7368(14)\text{ \AA}$	$\mu = 0.23\text{ mm}^{-1}$
$b = 5.2256(10)\text{ \AA}$	$T = 173\text{ K}$
$c = 28.619(4)\text{ \AA}$	$0.35 \times 0.08 \times 0.08\text{ mm}$
$\beta = 92.126(12)^\circ$	

#### Data collection

Oxford Diffraction Xcalibur Eos Gemini diffractometer	12731 measured reflections
Absorption correction: multi-scan ( <i>CrysAlis RED</i> ; Oxford Diffraction, 2010)	3460 independent reflections
	2206 reflections with $I > 2\sigma(I)$
	$R_{\text{int}} = 0.082$
	$T_{\min} = 0.925$ , $T_{\max} = 0.982$

#### Refinement

$R[F^2 > 2\sigma(F^2)] = 0.062$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.135$	$\Delta\rho_{\max} = 0.25\text{ e \AA}^{-3}$
$S = 1.05$	$\Delta\rho_{\min} = -0.36\text{ e \AA}^{-3}$
3460 reflections	
205 parameters	
2 restraints	

**Table 1**  
Hydrogen-bond geometry ( $\text{\AA}$ ,  $^\circ$ ).

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
N2—H2 $\cdots$ O1	0.86 (2)	1.85 (2)	2.600 (3)	144 (2)
N1—H1 $\cdots$ S1 <sup>i</sup>	0.86 (2)	2.80 (2)	3.591 (2)	153 (2)
C15—H15A $\cdots$ O1	0.95	2.51	3.411 (3)	159

Symmetry code: (i)  $-x + 1, -y + 1, -z + 1$ .

Data collection: *CrysAlis PRO* (Oxford Diffraction, 2010); cell refinement: *CrysAlis PRO*; data reduction: *CrysAlis RED* (Oxford Diffraction, 2010); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: FK2043).

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## **supplementary materials**

*Acta Cryst.* (2011). E67, o3187 [doi:10.1107/S160053681104582X]

### **1-Benzoyl-3-(naphthalen-1-yl)thiourea**

**S. Saeed, N. Rashid, J. P. Jasinski and J. A. Golen**

#### **Comment**

Thioureas are the subject of significant interest because of their usefulness in medicinal chemistry due to their biological activity as fungicides (Saeed *et al.*, 2010*a*), anticancer (Saeed *et al.*, 2010*b*), herbicides, rodenticides and phenoloxidase enzymatic inhibitors (Maddani & Prabhu, 2010). Recently, thiourea derivatives have found use in organocatalysis (Jung & Kim, 2008). Amino-thiourea derivatives (Saeed *et al.*, 2009) and their transition metal complexes are used as curing agents for epoxy resins (Saeed *et al.*, 2011). Thioureas have a long history as a ligand in coordination chemistry and coordinate readily to a metal *via* sulfur and oxygen (Burrows *et al.*, 1999). These hard and soft donor atoms provide a multitude of bonding possibilities (Henderson *et al.*, 2002). Hydrogen bonding behavior of some thioureas have been investigated and it is found that intramolecular hydrogen bonds between the carbonyl oxygen and a nitrogen atom is common. The complexing capacity of thiourea derivatives has been reported (Schuster *et al.*, 1990). Also, some acyl thioureas have been found to possess pesticidal activities and promote plant growth while others have been shown to have a notable positive effect on the germination of maize seeds and on the chlorophyll contents in seedling leaves (Che *et al.*, 1999). With the simultaneous presence of S, N and O electron donors, the versatility and behavior of acylthioureas as building blocks in polydentate ligands for metal ions have become a recent topic of interest. Substituted acylthiourea ligands might act as monodentate sulfur donors, bidentate oxygen and nitrogen donors. In continuation of our research program concerned with structural modification of biologically active thiourea derivatives and their transition metal complexes, we aim to incorporate the aliphatic and aromatic moieties in the substituted phenyl nucleus with thiourea functionality to obtain new functions in an attempt to improve the antimicrobial profile of these compounds. In view of the importance of thiourea derivatives, the crystal structure of the title compound, C<sub>18</sub>H<sub>14</sub>N<sub>2</sub>O<sub>8</sub>, (I), is reported.

In the title compound, (I), the dihedral angle between the mean planes of the 3-naphthyl and 1-benzoyl rings is 20.7 (1) $^{\circ}$  (Fig. 1). Crystal packing is stabilized by weak N1—H1···S1 intermolecular interactions (Table 1, Fig. 2). N2—H2···O1 intramolecular hydrogen bonds are also observed (Table 1).

#### **Experimental**

A solution of benzoyl chloride (0.01 mol) in anhydrous acetone (80 ml) and 3% tetrabutylammonium bromide (TBAB) as a phase-transfer catalyst (PTC) in anhydrous acetone was added dropwise to a suspension of dry ammonium thiocyanate (0.01 mol) in acetone (50 ml) and the reaction mixture was refluxed for 45 min. After cooling to room temperature, a solution of 1-naphthylamine (0.01 mol) in anhydrous acetone (25 ml) was added dropwise and the resulting mixture refluxed for 2.5 h. Hydrochloric acid (0.1 N, 300 ml) was added, and the solution was filtered. The solid product was washed with water and purified by re-crystallization from ethanol.

# supplementary materials

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## Refinement

All H atoms were positioned with idealized geometry using a riding model, [C—H = 0.95 Å and  $U_{\text{iso}} = 1.2U_{\text{eq}}(\text{C}, \text{N})$ ]. H(N) positions were refined freely.

## Figures

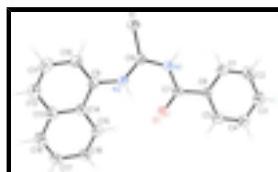


Fig. 1. Molecular structure of the title compound showing the atom labeling scheme and 50% probability displacement ellipsoids.

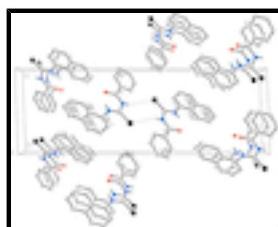


Fig. 2. Packing diagram of the title compound viewed along the  $b$  axis. Dashed lines indicate weak N1—H1···S1 intermolecular interactions.

## 1-Benzoyl-3-(naphthalen-1-yl)thiourea

### Crystal data

$\text{C}_{18}\text{H}_{14}\text{N}_2\text{OS}$	$F(000) = 640$
$M_r = 306.37$	$D_x = 1.398 \text{ Mg m}^{-3}$
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation, $\lambda = 0.71073 \text{ \AA}$
Hall symbol: -P 2yn	Cell parameters from 1307 reflections
$a = 9.7368 (14) \text{ \AA}$	$\theta = 3.5\text{--}32.3^\circ$
$b = 5.2256 (10) \text{ \AA}$	$\mu = 0.23 \text{ mm}^{-1}$
$c = 28.619 (4) \text{ \AA}$	$T = 173 \text{ K}$
$\beta = 92.126 (12)^\circ$	Rod, colourless
$V = 1455.2 (4) \text{ \AA}^3$	$0.35 \times 0.08 \times 0.08 \text{ mm}$
$Z = 4$	

### Data collection

Oxford Diffraction Xcalibur Eos Gemini diffractometer	3460 independent reflections
Radiation source: Enhance (Mo) X-ray Source graphite	2206 reflections with $I > 2\sigma(I)$
Detector resolution: 16.1500 pixels $\text{mm}^{-1}$	$R_{\text{int}} = 0.082$
$\omega$ scans	$\theta_{\text{max}} = 27.9^\circ, \theta_{\text{min}} = 4.0^\circ$
Absorption correction: multi-scan ( <i>CrysAlis RED</i> ; Oxford Diffraction, 2010)	$h = -12 \rightarrow 12$
$T_{\text{min}} = 0.925, T_{\text{max}} = 0.982$	$k = -6 \rightarrow 6$
	$l = -34 \rightarrow 37$

12731 measured reflections

### Refinement

Refinement on $F^2$	Primary atom site location: structure-invariant direct methods
Least-squares matrix: full	Secondary atom site location: difference Fourier map
$R[F^2 > 2\sigma(F^2)] = 0.062$	Hydrogen site location: inferred from neighbouring sites
$wR(F^2) = 0.135$	H atoms treated by a mixture of independent and constrained refinement
$S = 1.05$	$w = 1/[\sigma^2(F_o^2) + (0.0427P)^2 + 0.1745P]$ where $P = (F_o^2 + 2F_c^2)/3$
3460 reflections	$(\Delta/\sigma)_{\max} = 0.001$
205 parameters	$\Delta\rho_{\max} = 0.25 \text{ e } \text{\AA}^{-3}$
2 restraints	$\Delta\rho_{\min} = -0.36 \text{ e } \text{\AA}^{-3}$

### Special details

**Geometry.** All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

**Refinement.** Refinement of  $F^2$  against ALL reflections. The weighted  $R$ -factor  $wR$  and goodness of fit  $S$  are based on  $F^2$ , conventional  $R$ -factors  $R$  are based on  $F$ , with  $F$  set to zero for negative  $F^2$ . The threshold expression of  $F^2 > \sigma(F^2)$  is used only for calculating  $R$ -factors(gt) etc. and is not relevant to the choice of reflections for refinement.  $R$ -factors based on  $F^2$  are statistically about twice as large as those based on  $F$ , and  $R$ -factors based on ALL data will be even larger..

### Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ( $\text{\AA}^2$ )

	$x$	$y$	$z$	$U_{\text{iso}}^*/U_{\text{eq}}$
S1	0.63172 (7)	0.32704 (17)	0.54848 (3)	0.0446 (2)
O1	0.28206 (18)	0.5576 (4)	0.63936 (6)	0.0395 (5)
N1	0.4117 (2)	0.5657 (4)	0.57512 (7)	0.0300 (5)
H1	0.423 (3)	0.632 (5)	0.5480 (7)	0.036*
N2	0.4889 (2)	0.2542 (4)	0.62654 (7)	0.0280 (5)
H2	0.421 (2)	0.315 (5)	0.6413 (9)	0.034*
C1	0.2515 (3)	1.0084 (5)	0.54374 (9)	0.0313 (6)
H1A	0.3367	0.9825	0.5293	0.038*
C2	0.1632 (3)	1.1966 (5)	0.52738 (10)	0.0413 (7)
H2A	0.1872	1.2993	0.5016	0.050*
C3	0.0399 (3)	1.2359 (6)	0.54847 (11)	0.0427 (7)
H3A	-0.0216	1.3642	0.5369	0.051*
C4	0.0059 (3)	1.0899 (6)	0.58617 (10)	0.0407 (7)
H4A	-0.0784	1.1195	0.6010	0.049*
C5	0.0929 (3)	0.9015 (5)	0.60260 (10)	0.0364 (7)
H5A	0.0685	0.8010	0.6287	0.044*

## supplementary materials

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C6	0.2167 (2)	0.8566 (5)	0.58122 (8)	0.0257 (5)
C7	0.3049 (2)	0.6496 (5)	0.60124 (8)	0.0272 (6)
C8	0.5082 (2)	0.3745 (5)	0.58638 (9)	0.0292 (6)
C9	0.5611 (2)	0.0543 (5)	0.64982 (9)	0.0268 (6)
C10	0.6612 (2)	-0.0889 (5)	0.62991 (9)	0.0331 (6)
H10A	0.6876	-0.0526	0.5990	0.040*
C11	0.7248 (3)	-0.2889 (6)	0.65515 (10)	0.0395 (7)
H11A	0.7964	-0.3833	0.6415	0.047*
C12	0.6859 (3)	-0.3498 (5)	0.69861 (10)	0.0379 (7)
H12A	0.7289	-0.4890	0.7147	0.046*
C13	0.5827 (2)	-0.2094 (5)	0.72029 (9)	0.0297 (6)
C14	0.5195 (2)	-0.0002 (5)	0.69628 (8)	0.0261 (5)
C15	0.4192 (2)	0.1399 (5)	0.71991 (9)	0.0306 (6)
H15A	0.3758	0.2818	0.7048	0.037*
C16	0.3832 (3)	0.0759 (5)	0.76395 (9)	0.0354 (7)
H16A	0.3159	0.1740	0.7791	0.043*
C17	0.4444 (3)	-0.1323 (5)	0.78703 (9)	0.0371 (7)
H17A	0.4181	-0.1770	0.8176	0.045*
C18	0.5413 (3)	-0.2703 (5)	0.76558 (9)	0.0339 (6)
H18A	0.5826	-0.4119	0.7815	0.041*

### Atomic displacement parameters ( $\text{\AA}^2$ )

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
S1	0.0376 (4)	0.0694 (6)	0.0275 (4)	0.0166 (4)	0.0126 (3)	0.0087 (4)
O1	0.0407 (11)	0.0504 (12)	0.0283 (11)	0.0153 (10)	0.0124 (8)	0.0099 (9)
N1	0.0283 (11)	0.0381 (13)	0.0239 (12)	0.0030 (10)	0.0044 (9)	0.0055 (10)
N2	0.0248 (11)	0.0373 (13)	0.0223 (11)	0.0044 (10)	0.0066 (9)	0.0002 (9)
C1	0.0320 (14)	0.0316 (15)	0.0304 (15)	-0.0021 (12)	0.0043 (11)	-0.0020 (12)
C2	0.0535 (18)	0.0349 (16)	0.0356 (16)	0.0020 (14)	0.0032 (14)	0.0069 (13)
C3	0.0403 (16)	0.0390 (17)	0.0485 (19)	0.0075 (14)	-0.0042 (14)	0.0044 (14)
C4	0.0312 (15)	0.0450 (18)	0.0460 (18)	0.0060 (14)	0.0049 (13)	0.0053 (14)
C5	0.0315 (14)	0.0396 (17)	0.0384 (16)	0.0038 (13)	0.0063 (12)	0.0069 (13)
C6	0.0249 (13)	0.0277 (14)	0.0245 (13)	-0.0005 (11)	0.0015 (10)	-0.0014 (11)
C7	0.0261 (13)	0.0317 (14)	0.0241 (13)	-0.0010 (11)	0.0055 (10)	-0.0017 (11)
C8	0.0233 (13)	0.0381 (16)	0.0260 (14)	0.0033 (12)	0.0009 (10)	-0.0009 (12)
C9	0.0237 (12)	0.0276 (14)	0.0289 (14)	-0.0001 (11)	0.0003 (10)	-0.0024 (11)
C10	0.0285 (14)	0.0390 (16)	0.0319 (15)	0.0033 (12)	0.0017 (11)	-0.0021 (12)
C11	0.0312 (15)	0.0408 (17)	0.0463 (18)	0.0070 (13)	-0.0002 (13)	-0.0087 (14)
C12	0.0376 (15)	0.0348 (16)	0.0409 (17)	0.0019 (13)	-0.0050 (13)	0.0004 (13)
C13	0.0276 (13)	0.0270 (14)	0.0340 (15)	-0.0040 (11)	-0.0040 (11)	-0.0003 (11)
C14	0.0258 (13)	0.0260 (13)	0.0263 (14)	-0.0058 (11)	-0.0010 (10)	-0.0011 (10)
C15	0.0305 (14)	0.0312 (14)	0.0301 (14)	0.0025 (12)	0.0022 (11)	0.0024 (11)
C16	0.0394 (15)	0.0372 (16)	0.0302 (15)	0.0005 (13)	0.0074 (12)	0.0024 (12)
C17	0.0410 (16)	0.0426 (17)	0.0279 (15)	-0.0078 (14)	0.0029 (12)	0.0076 (13)
C18	0.0381 (15)	0.0286 (14)	0.0342 (15)	-0.0080 (13)	-0.0083 (12)	0.0053 (12)

*Geometric parameters (Å, °)*

S1—C8	1.667 (2)	C6—C7	1.483 (3)
O1—C7	1.220 (3)	C9—C10	1.370 (3)
N1—C7	1.375 (3)	C9—C14	1.433 (3)
N1—C8	1.401 (3)	C10—C11	1.401 (4)
N1—H1	0.859 (16)	C10—H10A	0.9500
N2—C8	1.329 (3)	C11—C12	1.351 (4)
N2—C9	1.412 (3)	C11—H11A	0.9500
N2—H2	0.861 (16)	C12—C13	1.407 (4)
C1—C2	1.377 (4)	C12—H12A	0.9500
C1—C6	1.386 (3)	C13—C18	1.408 (4)
C1—H1A	0.9500	C13—C14	1.419 (3)
C2—C3	1.379 (4)	C14—C15	1.413 (3)
C2—H2A	0.9500	C15—C16	1.362 (3)
C3—C4	1.372 (4)	C15—H15A	0.9500
C3—H3A	0.9500	C16—C17	1.395 (4)
C4—C5	1.370 (4)	C16—H16A	0.9500
C4—H4A	0.9500	C17—C18	1.353 (4)
C5—C6	1.392 (3)	C17—H17A	0.9500
C5—H5A	0.9500	C18—H18A	0.9500
C7—N1—C8	128.1 (2)	C10—C9—N2	123.9 (2)
C7—N1—H1	119.1 (18)	C10—C9—C14	120.5 (2)
C8—N1—H1	112.8 (18)	N2—C9—C14	115.6 (2)
C8—N2—C9	132.4 (2)	C9—C10—C11	120.0 (3)
C8—N2—H2	112.6 (18)	C9—C10—H10A	120.0
C9—N2—H2	115.0 (18)	C11—C10—H10A	120.0
C2—C1—C6	120.3 (2)	C12—C11—C10	121.1 (3)
C2—C1—H1A	119.9	C12—C11—H11A	119.5
C6—C1—H1A	119.9	C10—C11—H11A	119.5
C1—C2—C3	120.1 (3)	C11—C12—C13	120.8 (3)
C1—C2—H2A	120.0	C11—C12—H12A	119.6
C3—C2—H2A	120.0	C13—C12—H12A	119.6
C4—C3—C2	120.0 (3)	C12—C13—C18	121.4 (2)
C4—C3—H3A	120.0	C12—C13—C14	119.5 (2)
C2—C3—H3A	120.0	C18—C13—C14	119.1 (2)
C5—C4—C3	120.4 (3)	C15—C14—C13	117.5 (2)
C5—C4—H4A	119.8	C15—C14—C9	124.4 (2)
C3—C4—H4A	119.8	C13—C14—C9	118.1 (2)
C4—C5—C6	120.3 (3)	C16—C15—C14	121.4 (2)
C4—C5—H5A	119.9	C16—C15—H15A	119.3
C6—C5—H5A	119.9	C14—C15—H15A	119.3
C1—C6—C5	119.0 (2)	C15—C16—C17	120.7 (3)
C1—C6—C7	124.2 (2)	C15—C16—H16A	119.7
C5—C6—C7	116.8 (2)	C17—C16—H16A	119.7
O1—C7—N1	121.8 (2)	C18—C17—C16	119.6 (3)
O1—C7—C6	120.7 (2)	C18—C17—H17A	120.2
N1—C7—C6	117.5 (2)	C16—C17—H17A	120.2

## supplementary materials

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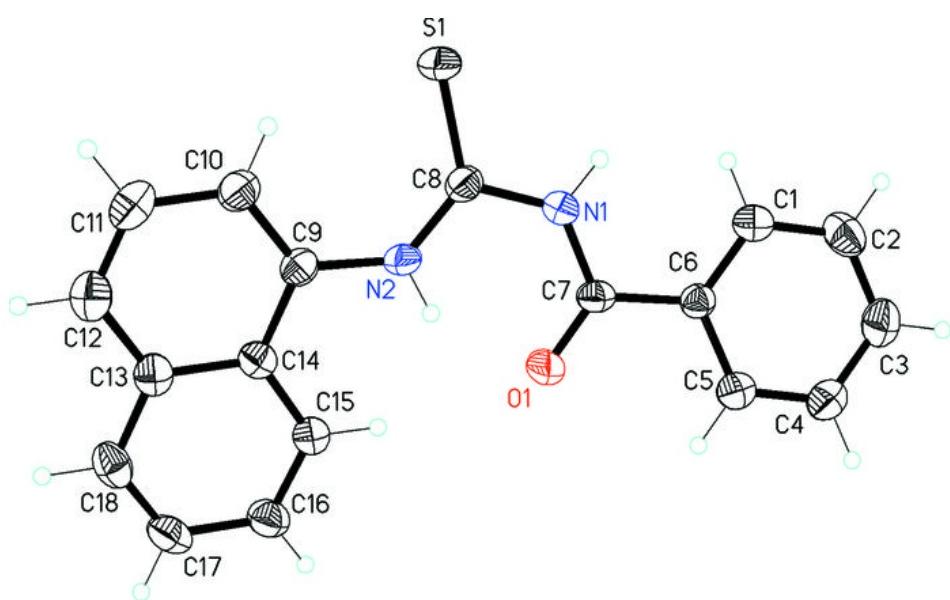
N2—C8—N1	114.9 (2)	C17—C18—C13	121.7 (3)
N2—C8—S1	128.4 (2)	C17—C18—H18A	119.2
N1—C8—S1	116.76 (19)	C13—C18—H18A	119.2
C6—C1—C2—C3	0.4 (4)	C14—C9—C10—C11	-0.6 (4)
C1—C2—C3—C4	0.9 (5)	C9—C10—C11—C12	2.2 (4)
C2—C3—C4—C5	-1.1 (5)	C10—C11—C12—C13	-1.7 (4)
C3—C4—C5—C6	0.1 (4)	C11—C12—C13—C18	-179.9 (2)
C2—C1—C6—C5	-1.5 (4)	C11—C12—C13—C14	-0.5 (4)
C2—C1—C6—C7	180.0 (2)	C12—C13—C14—C15	-178.2 (2)
C4—C5—C6—C1	1.2 (4)	C18—C13—C14—C15	1.2 (3)
C4—C5—C6—C7	179.9 (2)	C12—C13—C14—C9	2.0 (3)
C8—N1—C7—O1	-0.4 (4)	C18—C13—C14—C9	-178.6 (2)
C8—N1—C7—C6	180.0 (2)	C10—C9—C14—C15	178.8 (2)
C1—C6—C7—O1	165.4 (3)	N2—C9—C14—C15	-3.5 (4)
C5—C6—C7—O1	-13.2 (4)	C10—C9—C14—C13	-1.5 (3)
C1—C6—C7—N1	-15.0 (4)	N2—C9—C14—C13	176.2 (2)
C5—C6—C7—N1	166.4 (2)	C13—C14—C15—C16	-0.5 (4)
C9—N2—C8—N1	179.7 (2)	C9—C14—C15—C16	179.2 (2)
C9—N2—C8—S1	-0.6 (4)	C14—C15—C16—C17	-0.4 (4)
C7—N1—C8—N2	3.1 (4)	C15—C16—C17—C18	0.7 (4)
C7—N1—C8—S1	-176.7 (2)	C16—C17—C18—C13	0.0 (4)
C8—N2—C9—C10	-10.9 (4)	C12—C13—C18—C17	178.4 (3)
C8—N2—C9—C14	171.5 (3)	C14—C13—C18—C17	-0.9 (4)
N2—C9—C10—C11	-178.1 (2)		

*Hydrogen-bond geometry (Å, °)*

<i>D</i> —H··· <i>A</i>	<i>D</i> —H	H··· <i>A</i>	<i>D</i> ··· <i>A</i>	<i>D</i> —H··· <i>A</i>
N2—H2···O1	0.86 (2)	1.85 (2)	2.600 (3)	144 (2)
N1—H1···S1 <sup>i</sup>	0.86 (2)	2.80 (2)	3.591 (2)	153 (2)
C15—H15A···O1	0.95	2.51	3.411 (3)	159.

Symmetry codes: (i)  $-x+1, -y+1, -z+1$ .

Fig. 1



## supplementary materials

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Fig. 2

